1

Gasphase Energy: -1274.120316 Hartrees

Solvation Phase Energy: -1274.130824 Hartrees

Zero Point Energy: 218.85 kcal/mol

Coordinates:

Ru1	-2.5403591011	1.4703168724	-0.1221544876
N2	-2.5198282743	3.6641895728	-0.2802127892
N3	-4.6414190083	1.6781784656	-0.2080846867
N4	-2.6099338773	1.5615820159	-2.3908787826
N5	-5.1884656786	2.5455763102	-1.1062813812
N6	-3.3421214590	4.2568627702	-1.1876100226
N7	-3.4660821731	2.4550020222	-2.9523567404
B8	-4.3017897957	3.3988389906	-2.0538887928
C9	-1.8347118831	4.6376727327	0.3281370389
C10	-5.6483720345	1.1177330022	0.4715530876
C11	-2.0368933256	0.8902450779	-3.3941334481
C12	-3.4267861994	2.3440349062	-4.3010932534
C13	-3.1694297931	5.5976266838	-1.1460528713
C14	-6.5357668332	2.5226433463	-0.9827803087
H15	-4.9938276508	4.1089218238	-2.7294618601
C16	-6.8753409109	1.6197821869	0.0141391656
C17	-2.5190611329	1.3488347585	-4.6318151481
C18	-2.2079319687	5.8888448464	-0.1882303989
H19	-1.1385989381	4.3909482435	1.1165027139
H20	-5.4365827481	0.4031470198	1.2526469753
H21	-1.3148813413	0.1145345890	-3.1803150864
H22	-4.0430186263	2.9783981908	-4.9207715088
H23	-3.7445268998	6.2422240137	-1.7939494125
H24	-7.1492541182	3.1500874019	-1.6116480022
H25	-7.8636691273	1.3628294984	0.3625941665
H26	-2.2484891486	1.0043686550	-5.6182237360
H27	-1.8409847433	6.8613752586	0.1019323429
O28	-2.7302064069	-1.5417176841	0.1028198003
C29	-2.6496294295	-0.3886664764	0.0089305530
C30	-2.5061854976	1.9149802136	4.8030802085
C31	-3.3494877294	2.6991667821	4.0147321964
C32	-3.3665292605	2.5465831771	2.6242914107
C33	-2.5435743427	1.6118151349	1.9661422313
C34	-1.7049908380	0.8333203310	2.7890342782
C35	-1.6822870644	0.9764837480	4.1796370583
H36	-2.4944665612	2.0297309232	5.8837966568
H37	-4.0009180085	3.4350776194	4.4814915245
H38	-4.0349125369	3.1758435702	2.0437721735
H39	-1.0533999122	0.0865366343	2.3391696369
H40	-1.0215462637	0.3503651343	4.7758263481
C41	0.6597883557	1.4984576603	0.0221268109
N42	-0.4939408227	1.4560276655	-0.0675024034
C43	2.1094174550	1.5596867969	0.1586952568
H44	2.3792390966	2.2444593398	0.9668754829
H45	2.5057121242	0.5688131337	0.3940329573
H46	2.5658165298	1.9110343515	-0.7699393937

2

Gasphase Energy: -232.253110 Hartrees
Solvation Phase Energy: -232.254952 Hartrees
Zero Point Energy: 63.16 kcal/mol
Coordinates:

C1	2.5031320127	-.0490056072	-.0000194456
C2	1.8050967939	1.1600216456	-.0000165615
C3	.4090203225	1.1600253222	.0000113247
C4	-.2890116689	-.0489988352	.0000613738
C5	.4090221090	-1.2580267594	.0000105218
C6	1.8050984190	-1.2580311214	-.0000170636
H7	3.5893141016	-.0490041585	-.0000408448
H8	2.3481908968	2.1006718658	-.0000534579
H9	-.1340755133	2.1006739675	-.0000567426
H10	-1.3751937138	-.0490080623	-.0000984192
H11	-.1340699578	-2.1986772876	-.0000555320
H12	2.3481890716	-2.1986832549	-.0000539900

3

Gasphase Energy: -78.591974 Hartrees
Solvation Phase Energy: -78.593306 Hartrees
Zero Point Energy: 32.07 kcal/mol
Coordinates:

C1	0.0692912927	1.1652498267	0.0000000642
C2	-1.2615173253	1.1652500062	-0.0000001092
H3	0.6418584277	0.2413097856	0.0000001087
H4	-1.8340840859	0.2413097708	0.0000001595
H5	-1.8340859165	2.0891886343	0.0000001559
H6	0.6418599624	2.0891884949	0.0000001124

4

Gasphase Energy: -310.886555 Hartrees
Solvation Phase Energy: -310.888372 Hartrees
Zero Point Energy: 98.60 kcal/mol
Coordinates:

C1	2.5115750000	-0.0490040000	0.0000000000
C2	1.8092750000	1.1673960000	0.0000000000
C3	0.4047750000	1.1673960000	0.0000000000
C4	-0.2974250000	-0.0490040000	0.0000000000
C5	0.4047750000	-1.2654040000	0.0000000000
C6	1.8093750000	-1.2654040000	0.0000000000
H7	3.6149750000	-0.0490040000	0.0000000000
H8	2.3610750000	2.1229960000	0.0000000000
H9	-0.1469250000	2.1229960000	0.0000000000
H10	-0.1469250000	-2.2209040000	0.0000000000
H11	2.3610750000	-2.2210040000	0.0000000000
C12	-1.8194250000	-0.0490040000	0.0000000000
H13	-2.1923900000	0.4784490000	0.9135750000
H14	-2.1923900000	0.4784490000	-0.9135750000
C15	-2.3280920000	-1.4877310000	0.0000000000
H16	-1.9551260000	-2.0151830000	-0.9135750000
H17	-1.9551260000	-2.0151830000	0.9135750000
H18	-3.4469880000	-1.4877310000	0.0000000000

5

Gasphase Energy: -1141.321859 Hartrees
Solvation Phase Energy: -1141.329540 Hartrees
Zero Point Energy: 188.99 kcal/mol
Coordinates:

Ru1	-2.6745074991	1.4445492593	-0.0748420885
N2	-2.5326360999	3.6045377473	-0.2236761475
N3	-4.6845674917	1.6880812323	-0.2751637586
N4	-2.5795347206	1.5059369500	-2.3393593346
N5	-5.1555921611	2.5759384414	-1.1961621677
N6	-3.2631401020	4.2334627950	-1.1842386859
N7	-3.3517479421	2.4396413389	-2.9560311479
B8	-4.1990887366	3.4094584402	-2.1040648945
C9	-1.8414613148	4.5463171751	0.4304479935
C10	-5.7353969092	1.1585196219	0.3655431968
C11	-1.9733320597	0.8062437432	-3.3044343392
C12	-3.2270247046	2.3260026238	-4.2991349159
C13	-3.0253622872	5.5634069057	-1.1328157531
C14	-6.5062630968	2.5974879601	-1.1252751646
H15	-4.8428144085	4.1370644267	-2.8062648744
C16	-6.9197132464	1.7067418521	-0.1452479811
C17	-2.3473898952	1.2885471068	-4.5699310141
C18	-2.1141202372	5.8097471446	-0.1147538631
H19	-1.2117186349	4.2701698185	1.2632970487
H20	-5.5796638778	0.4356587367	1.1516791279
H21	-1.3069079971	-0.0055622618	-3.0475117090
H22	-3.7705551443	2.9865296523	-4.9582727859
H23	-3.5221330516	6.2343072573	-1.8179300409
H24	-7.0705774831	3.2464283355	-1.7776645005
H25	-7.9304044289	1.4857696272	0.1606893295
H26	-2.0269471250	0.9314742659	-5.5365598116
H27	-1.7143760638	6.7630151786	0.1945994492
O28	-2.9934220215	-1.5654714465	0.1489135437
C29	-2.8490002385	-0.4194472623	0.0560156021
C30	-2.2999295882	1.9568247283	4.7869310613
C31	-3.2664267325	2.6841053260	4.0876506415
C32	-3.4240651977	2.5079762773	2.7105638287
C33	-2.6296424159	1.5992651198	1.9848996297
C34	-1.6777284746	0.8620797720	2.7185821310
C35	-1.5019576266	1.0453050093	4.0942852517
H36	-2.1770825031	2.0923441656	5.8580993346
H37	-3.8984913598	3.3946141340	4.6158184260
H38	-4.1756097129	3.0971786104	2.1916386344
H39	-1.0587445284	0.1182622581	2.2168000415
H40	-0.7523176568	0.4629969289	4.6250251766

6

Gasphase Energy: -1219.951597 Hartrees
Solvation Phase Energy: -1219.958609 Hartrees
Zero Point Energy: 223.95 kcal/mol
Coordinates:

Ru1	-2.4184739896	1.5125597271	-0.1206001402
N2	-2.4662740509	3.7259748643	-0.3286717763
N3	-4.5654914562	1.6410517322	-0.1437774340
N4	-2.6808420265	1.5492672292	-2.3825033476
N5	-5.1825238800	2.5152663748	-0.9852105533
N6	-3.3760322446	4.2677526753	-1.1864493890
N7	-3.5706456401	2.4305685065	-2.9090502555
B8	-4.3669507457	3.3780334608	-1.9813904878
C9	-1.7743068629	4.7454813418	0.1962571170
C10	-5.5184926856	1.0280554977	0.5677011499
C11	-2.1939700745	0.8329723667	-3.4018087776
C12	-3.6382300834	2.2673735183	-4.2508530767
C13	-3.2474569021	5.6137111370	-1.1952061316
C14	-6.5205006496	2.4422167948	-0.8004355447
H15	-5.1049800348	4.0681661683	-2.6269890541
C16	-6.7815856522	1.5013894247	0.1856885875
C17	-2.7674752196	1.2503963635	-4.6131798910
C18	-2.2286964072	5.9665359470	-0.3220925914
H19	-1.0056476752	4.5616865301	0.9321391330
H20	-5.2455881841	0.3057724900	1.3224469953
H21	-1.4626850348	0.0580882494	-3.2214401865
H22	-4.2975483706	2.8837468195	-4.8436103153
H23	-3.8899203341	6.2182292772	-1.8177829131
H24	-7.1840657759	3.0627685864	-1.3838778626
H25	-7.7426647624	1.2034673765	0.5753021848
H26	-2.5757669203	0.8666004980	-5.6033892904
H27	-1.8719097789	6.9578994441	-0.0891174597
O28	-2.4380186714	-1.5041172118	-0.0518745544
C29	-2.4309406777	-0.3449832758	-0.0606660095
C30	-0.2621382611	1.5747654639	-0.7691360202
C31	-0.2799691581	1.6316347220	0.6147334773
H32	-0.0231108684	0.6482400403	-1.2809375417
H33	-0.0670108420	0.7540543091	1.2132787967
H34	-0.1804691433	2.5724126464	1.1422460360
H35	-0.1783873222	2.4776782981	-1.3637247121
X36	-0.4742280869	1.5709608672	-0.0247244879
C37	-3.0482870333	1.7634191736	4.8054727071
C38	-3.4590650253	2.7934310100	3.9587663883
C39	-3.2540154805	2.7045361950	2.5777325197
C40	-2.6240669467	1.5915772934	1.9907872205
C41	-2.2263188947	0.5640774283	2.8675053874
C42	-2.4332365158	0.6421186150	4.2482979854
H43	-3.2070257953	1.8315687632	5.8782640069
H44	-3.9470333773	3.6742102630	4.3702351293
H45	-3.6036939634	3.5195327145	1.9528637398
H46	-1.7382215466	-0.3269505141	2.4792041965
H47	-2.1097399892	-0.1776705093	4.8857475177

7

Gasphase Energy: -1219.957559 Hartrees
Solvation Phase Energy: -1219.964251 Hartrees
Zero Point Energy: 224.64 kcal/mol
Coordinates:

Ru1	-2.4933520457	1.3351131945	-0.2350469563
N2	-2.4040799771	3.5684394949	-0.2529186102
N3	-4.5390361339	1.6319598914	-0.1418951493
N4	-2.6909216110	1.5619402616	-2.4912859839
N5	-5.1322947574	2.5403920906	-0.9647573515
N6	-3.2695276556	4.2145207943	-1.0819778336
N7	-3.5487366127	2.5171768656	-2.9392244585
B8	-4.2950159007	3.4211553828	-1.9343707963
C9	-1.7103918053	4.5160461115	0.3918298899
C10	-5.4994074980	1.0756361123	0.6064153910
C11	-2.2111551157	0.9366577386	-3.5708125908
C12	-3.6006802668	2.4918726309	-4.2926799039
C13	-3.1148462691	5.5518093168	-0.9543438268
C14	-6.4639904640	2.5513947482	-0.7239533686
H15	-5.0179786728	4.1810288369	-2.5168126095
C16	-6.7446971593	1.6269065584	0.2711136172
C17	-2.7544123066	1.4902886251	-4.7431940314
C18	-2.1186583492	5.7936050637	-0.0199569172
H19	-0.9652703231	4.2406163739	1.1237781949
H20	-5.2450563405	0.3195464495	1.3338793170
H21	-1.5061795347	0.1260295347	-3.4524414044
H22	-4.2331606458	3.1830970955	-4.8297420769
H23	-3.7253068811	6.2289164284	-1.5329476996
H24	-7.1088541477	3.2173114305	-1.2772652968
H25	-7.7072662255	1.3852838319	0.6945380873
H26	-2.5616383771	1.2006210386	-5.7649094116
H27	-1.7473304450	6.7487277966	0.3180286386
O28	-2.9061468077	-1.6513806667	-0.1779488041
C29	-2.7143599295	-0.5052939541	-0.2125802538
C30	-2.2587736003	1.3595438314	1.8880415749
H31	-2.7202630819	0.4900377783	2.3683716025
H32	-2.7377679415	2.2571529402	2.2931527891
C33	-0.7376051138	1.3619588561	2.1590627961
H34	-0.4697658340	0.8633116513	3.1000957505
H35	-0.3606197068	2.3894259025	2.2358831004
C36	1.0738883631	-0.6298886971	-1.2489725001
C37	0.6837381530	0.7003532946	-1.3426405070
C38	0.1328637426	1.3596440636	-0.2275783282
C39	-0.0471787019	0.6765601338	0.9946713481
C40	0.3654941786	-0.6664782968	1.0707386310
C41	0.9218611949	-1.3074510585	-0.0306121578
H42	1.5063693030	-1.1380367073	-2.1056408412
H43	0.8174382197	1.2495366449	-2.2698562473
H44	-0.0412070380	2.4298584475	-0.2833058197
H45	0.2410316682	-1.2045442749	2.0065934323
H46	1.2389155255	-2.3432883831	0.0537940086

8

Gasphase Energy: -1219.947580 Hartrees
Solvation Phase Energy: -1219.955293 Hartrees
Zero Point Energy: 224.34 kcal/mol
Coordinates:

Ru1	-2.6125058404	1.6306039041	-0.0916656954
N2	-2.7424473846	3.7971649062	-0.3251718047
N3	-4.6390131619	1.6002326842	-0.2794864468
N4	-2.5246698956	1.6350018170	-2.3707940542
N5	-5.2255702531	2.3912013481	-1.2221297765
N6	-3.5664273895	4.2833514688	-1.2925874738
N7	-3.4301622488	2.4307696840	-3.0013158599
B8	-4.3918554298	3.3070350096	-2.1696337265
C9	-2.1767205667	4.8517827162	0.2756305380
C10	-5.6099921850	0.9480468575	0.3727672942
C11	-1.8381793101	0.9998721514	-3.3262053729
C12	-3.3067981117	2.2955547738	-4.3429996984
C13	-3.5141478592	5.6341410054	-1.2959147600
C14	-6.5672744034	2.2312875279	-1.1503262824
H15	-5.1315410789	3.9187534827	-2.8880888348
C16	-6.8576378430	1.3172982677	-0.1482349876
C17	-2.2926564894	1.3852049494	-4.5988913751
C18	-2.6297407268	6.0443019854	-0.3076333741
H19	-1.4886928004	4.7033307235	1.0956105876
H20	-5.3607299954	0.2644337695	1.1698318553
H21	-1.0604189418	0.2984244460	-3.0575491888
H22	-3.9471168752	2.8520430919	-5.0113174488
H23	-4.1088878693	6.2021165821	-1.9956784737
H24	-7.2129470007	2.7806184438	-1.8185467886
H25	-7.8292116052	0.9679733670	0.1646869462
H26	-1.9379178396	1.0468627314	-5.5603238701
H27	-2.3579622954	7.0548103739	-0.0444795311
O28	-2.5357414117	-1.3693198330	0.3136995231
C29	-2.5434569725	-0.2212142156	0.1386611725
C30	-2.6420828493	1.8832368665	2.0095939728
H31	-3.2980980818	1.1728720780	2.5267789399
H32	-3.0324821010	2.8854517449	2.2227959361
C33	-1.2100085676	1.7506395775	2.5724632950
H34	-0.5204000741	2.4074668239	2.0186941899
H35	-0.8475848821	0.7254238881	2.4223302120
C36	-1.0250782397	2.7353048649	6.7925786188
C37	-1.3354280515	1.4367813016	6.3827466606
C38	-1.3786344457	1.1213976436	5.0243920423
C39	-1.1137169617	2.0928822720	4.0487263056
C40	-0.8011482059	3.3904503789	4.4747020208
C41	-0.7572052253	3.7122131985	5.8321806547
H42	-0.9882226868	2.9818772303	7.8498925638
H43	-1.5395209025	0.6670223498	7.1222143879
H44	-1.6166980808	0.1067720752	4.7130906839
H45	-0.5840975298	4.1572169480	3.7338378786
H46	-0.5092035939	4.7246493506	6.1394895465

9

Gasphase Energy: -1452.210791 Hartrees
Solvation Phase Energy: -1452.218899 Hartrees
Zero Point Energy: 288.34 kcal/mol
Coordinates:

Ru1	-2.6944703642	1.7332028029	-0.1537139843
N2	-2.8505214683	3.8996759204	-0.5468863599
N3	-4.7561706487	1.7677069692	-0.0306731369
N4	-2.9914815988	1.5523440853	-2.4063029318
N5	-5.4708145412	2.4849658306	-0.9426696068
N6	-3.8122604662	4.3165978396	-1.4147841108
N7	-3.9641510480	2.3233828321	-2.9631157262
B8	-4.7747868104	3.2928201212	-2.0757256477
C9	-2.2017381934	4.9944790305	-0.1279547484
C10	-5.6294295958	1.1897892960	0.8041578553
C11	-2.4609567009	0.8241025976	-3.3930493550
C12	-4.0401882768	2.0776671574	-4.2931787779
C13	-3.7625809012	5.6623941789	-1.5369075173
C14	-6.7897081127	2.3544033946	-0.6699496079
H15	-5.6004690987	3.8678275962	-2.7281111068
C16	-6.9381841032	1.5326226117	0.4372723715
C17	-3.0907374021	1.1195688150	-4.6146185890
C18	-2.7393471222	6.1416993411	-0.7311457358
H19	-1.3953879277	4.9070263210	0.5862649375
H20	-5.2746195255	0.5659349203	1.6102563558
H21	-1.6561968661	0.1345647810	-3.1807438367
H22	-4.7606172408	2.5984062669	-4.9065289370
H23	-4.4582747169	6.1774254218	-2.1824385878
H24	-7.5213492592	2.8553025510	-1.2856422229
H25	-7.8565589626	1.2250013323	0.9125703954
H26	-2.8856616473	0.6954921690	-5.5857153541
H27	-2.4331230148	7.1672002476	-0.5936634224
O28	-2.6974429416	-1.2429588395	0.3689479442
C29	-2.6696544527	-0.0984981440	0.1680113577
C30	-2.5166666372	2.1434338887	1.9453986112
H31	-3.5082716914	2.0435919066	2.4038338272
H32	-2.2540038599	3.2064051293	2.0368763120
C33	-1.5058001531	1.3094829668	2.7622953784
H34	-0.5119257265	1.3528891869	2.2973254803
H35	-1.8040186252	0.2538432597	2.7475775163
C36	-1.1509521253	2.6452592242	6.8719879390
C37	-2.1163676497	1.6995041342	6.5201186936
C38	-2.2233049943	1.2652359241	5.1984338307
C39	-1.3721648993	1.7635682105	4.2023287466
C40	-0.4078682290	2.7117406086	4.5710258623
C41	-0.2957743407	3.1507135120	5.8908730215
H42	-1.0623935151	2.9807583094	7.9014507292
H43	-2.7824682048	1.2943600824	7.2772834077
H44	-2.9717727069	0.5216111363	4.9332577269
H45	0.2685833402	3.1025586772	3.8135014566
H46	0.4640407653	3.8818061782	6.1544732052
C47	0.5279761793	0.5347148399	-0.4447105453
C48	-0.0994770587	1.7772144798	-0.5963462170
H49	0.2695614555	-0.1023925507	0.3945865492
H50	-0.7421046182	2.1570672165	0.2248276346
X51	-0.3191567369	1.5578181861	-0.1054602026

C52	1.8187291636	0.9586350089	-2.4442503869
C53	1.4845238886	0.1241771523	-1.3740485012
H54	2.5647385461	0.6391979072	-3.1664326922
H55	1.9693276746	-0.8410707267	-1.2625899639
C56	1.2030113768	2.2057701361	-2.5846691303
C57	0.2423967321	2.6182396221	-1.6612560525
H58	1.4681314051	2.8527519644	-3.4154772216
H59	-0.2494475818	3.5787353670	-1.7681641478

10

Gasphase Energy: -1452.216535 Hartrees
Solvation Phase Energy: -1452.224588 Hartrees
Zero Point Energy: 288.27 kcal/mol
Coordinates:

Ru1	-1.6390503335	-1.2718473439	-0.8537321237
N2	-0.9367194547	-0.9337349391	1.1895531587
N3	-0.3961905554	-3.1731410538	-0.7199032420
N4	-3.1574575756	-2.3452508139	0.0117906005
N5	-0.5146368364	-3.8968599184	0.4253890160
N6	-0.9117137979	-1.9957207670	2.0410489828
N7	-2.8700685388	-3.2072886120	1.0281670026
B8	-1.4193480685	-3.3832864758	1.5684681945
C9	-0.4974873570	0.1301541163	1.8732036728
C10	0.4271340383	-3.8541657716	-1.5243252603
C11	-4.4779418931	-2.3909412319	-0.2051717903
C12	-4.0188643451	-3.7892426589	1.4438681611
C13	-0.4533771284	-1.5961287858	3.2490952370
C14	0.2325626520	-5.0224202434	0.3374226337
H15	-1.4198220738	-4.1587485517	2.4826008763
C16	0.8584543866	-5.0364201451	-0.9000647178
C17	-5.0703051413	-3.2999759663	0.6822798274
C18	-0.1692804014	-0.2388472282	3.1865595486
H19	-0.4691775905	1.0997045367	1.3981872461
H20	0.6643580571	-3.4697578944	-2.5067580358
H21	-4.9203695011	-1.7648219548	-0.9647091411
H22	-4.0008776961	-4.5049953541	2.2517765482
H23	-0.3678552102	-2.3023422596	4.0614511529
H24	0.2627028831	-5.7252677121	1.1566711782
H25	1.5234494766	-5.7894259457	-1.2941239898
H26	-6.1154186936	-3.5567790409	0.7586501646
H27	0.2091945674	0.3921634360	3.9758335431
O28	-2.7358717518	-1.8369524597	-3.6204412309
C29	-2.2988309135	-1.6149877857	-2.5701622683
C30	0.5296825970	0.3471395773	-1.8079177063
H31	-0.1646014574	1.0852228486	-1.4072950642
H32	0.5766561766	0.4852437253	-2.8920870455
C33	1.9176265125	0.4618532535	-1.1530515844
H34	2.5848768768	-0.3007890247	-1.5698364365
H35	1.8230332911	0.2502176900	-0.0825881361
C36	3.5493216530	4.4217278639	-1.7858674518
C37	2.6952421541	4.1761526236	-0.7084463980
C38	2.1853731062	2.8949739132	-0.4982723891
C39	2.5160250395	1.8380782945	-1.3575435304
C40	3.3743594134	2.0972786353	-2.4334065797
C41	3.8885803850	3.3773352926	-2.6475973084

H42	3.9485714971	5.4184007071	-1.9507003606
H43	2.4277169249	4.9816149669	-0.0301599456
H44	1.5245386346	2.7104027396	0.3456946363
H45	3.6445116711	1.2874363626	-3.1073642964
H46	4.5553377073	3.5579201557	-3.4862502874
H47	0.1533815911	-0.6949642973	-1.6548769112
C48	-4.1116705023	2.9912725165	-0.5815762602
C49	-4.1170282273	2.0910206757	0.4852161186
C50	-3.4453682392	0.8684131205	0.3844103765
C51	-2.7396980568	0.4984442965	-0.7778831270
C52	-2.7713840657	1.4189717902	-1.8459788142
C53	-3.4356813555	2.6458751281	-1.7524475107
H54	-4.6307010476	3.9428424650	-0.5043581116
H55	-4.6439904112	2.3397044371	1.4038665666
H56	-3.4686109379	0.1942729404	1.2359101586
H57	-2.2640755171	1.1837006222	-2.7799051805
H58	-3.4263970449	3.3284819334	-2.5991953755

TS1

Gasphase Energy: -1219.917714 Hartrees
Solvation Phase Energy: -1219.924248 Hartrees
Zero Point Energy: 223.49 kcal/mol
Imaginary frequencies: -352.85 cm^{-1}
Coordinates:

Ru1	-0.0623750086	-0.0825472582	0.0154909358
N2	-0.0347844199	-0.0724245467	2.2542742711
N3	2.1553780578	0.1074778810	0.2030385831
N4	0.2896315036	-2.1766502321	0.2846447472
N5	2.7971299381	-0.6307825054	1.1475182333
N6	0.9525600578	-0.7739241445	2.8744837017
N7	1.2193952603	-2.6028385738	1.1811814886
B8	1.9977113857	-1.5860986849	2.0571159637
C9	-0.8206797043	0.4226608206	3.2199791981
C10	3.0787481623	0.8588636833	-0.4032889135
C11	-0.2392927111	-3.2649955212	-0.2874951271
C12	1.2651784407	-3.9549276592	1.1727689723
C13	0.7843465797	-0.7124472033	4.2148015663
C14	4.1201283132	-0.3404586042	1.1314982010
H15	2.7340356817	-2.1666243603	2.8053715484
C16	4.3470666440	0.6114948049	0.1489708188
C17	0.3480431460	-4.4232159756	0.2431983811
C18	-0.3419524791	0.0510824026	4.4849242553
H19	-1.6872957076	1.0167198639	2.9674041906
H20	2.7851043033	1.5422697400	-1.1872491694
H21	-1.0049663320	-3.1590338583	-1.0418451698
H22	1.9440103013	-4.4800229865	1.8278505160
H23	1.4749526054	-1.2167144044	4.8739524025
H24	4.7962133009	-0.8312193002	1.8158252583
H25	5.2886234631	1.0601584807	-0.1286941679
H26	0.1335394221	-5.4491718145	-0.0131724759
H27	-0.7561547030	0.3005148461	5.4496370525
O28	-0.0839013216	-0.5350161223	-2.9633344762
C29	-0.0681707966	-0.3210693682	-1.8208381942
C30	-2.1830183219	-0.0530360125	0.0950029558
C31	-1.9430480634	1.3828301497	0.0152700155

H32	-2.6943769883	-0.5057422394	-0.7523881515
H33	-2.3167252086	1.8733301229	-0.8781070247
H34	-2.1584228786	1.9644702768	0.9075245813
H35	-2.5200769262	-0.4464054955	1.0519438818
C36	1.1635963904	4.6288978738	-0.5518325692
C37	0.9636013960	4.1052031546	0.7279299308
C38	0.2874656296	2.8978998108	0.9011765586
C39	-0.1903185257	2.1582701336	-0.1998890100
C40	-0.0062529009	2.7249086702	-1.4801445398
C41	0.6691681777	3.9315632951	-1.6573512291
H42	1.6825293158	5.5738190480	-0.6851471931
H43	1.3347813846	4.6390795922	1.5986553690
H44	0.1466635183	2.5149823507	1.9060547829
H45	-0.4083822486	2.2186178603	-2.3533338003
H46	0.7984834112	4.3319665339	-2.6596375097

TS2

Gasphase Energy: -1452.178668 Hartrees
Solvation Phase Energy: -1452.186275 Hartrees
Zero Point Energy: 285.87 kcal/mol
Imaginary frequencies: -1137.17 cm^{-1}
Coordinates:

Ru1	-.1319293883	-.0180283147	-.0303528805
N2	-.0129487910	.0256054963	2.1851214513
N3	2.0611932575	.1022929580	.0783443219
N4	.1891298499	-2.1680735255	.2157694018
N5	2.7200922465	-.6616855188	.9874079682
N6	.9578743675	-.7184254194	2.7858904511
N7	1.1119361657	-2.6026836536	1.1168417337
B8	1.9356110442	-1.5886720592	1.9492505436
C9	-.6845723420	.6489204241	3.1623512509
C10	2.9840504458	.8024491533	-.5916764574
C11	-.3800706435	-3.2511244297	-.3233954410
C12	1.1173704697	-3.9559414455	1.1385196389
C13	.8899681649	-.5566404317	4.1265550137
C14	4.0509761048	-.4388497608	.8887123558
H15	2.6927073006	-2.1675520527	2.6770253714
C16	4.2674446654	.4953736171	-.1139153732
C17	.1761764226	-4.4155805068	.2287159997
C18	-.1511587850	.3141377402	4.4153870460
H19	-1.5225543517	1.2858623217	2.9211232584
H20	2.6836926859	1.4855040647	-1.3733068688
H21	-1.1572596554	-3.1375264376	-1.0650514975
H22	1.7880421561	-4.4882797315	1.7964832531
H23	1.5838770309	-1.0726970317	4.7731184378
H24	4.7408710569	-.9593822127	1.5361024754
H25	5.2117975978	.8942987506	-.4507236883
H26	-.0718933761	-5.4401767604	-.0019615755
H27	-.4783060094	.6536145025	5.3860153195
O28	-.0286697275	-.1433798904	-3.0462473069
C29	-.0925870487	-.0951583719	-1.8901880337
C30	-.2585556534	2.2426504755	-.0815435898
H31	-.0175761092	2.5139600840	-1.1116212831
H32	.6193642471	2.4256214448	.5403862170
C33	-1.4134450524	3.1539071448	.4023366258

H34	-1.6555059154	2.9292865004	1.4475872818
H35	-2.3245970603	2.9643139303	-.1770557652
C36	-.2543773898	7.3085622731	.0115223686
C37	-1.0396957190	6.7031110006	-.9715171642
C38	-1.4255432868	5.3683073298	-.8358074766
C39	-1.0365132241	4.6163742954	.2804289499
C40	-.2502487855	5.2371799691	1.2614436672
C41	.1390789529	6.5702129767	1.1304683473
H42	.0463906698	8.3474165002	-.0913344316
H43	-1.3548585878	7.2702009587	-1.8435857849
H44	-2.0402724168	4.9026577399	-1.6033114921
H45	.0585455925	4.6676607868	2.1353779515
H46	.7474870948	7.0338320316	1.9029069141
H47	-1.3578069992	1.0196398794	.0440993488
C48	-5.0456196218	-.8923134528	-.1459693283
C49	-4.2707132654	-1.2138288214	.9707103368
C50	-2.9160472739	-.8781504943	1.0156284530
C51	-2.2879580970	-.2259880295	-.0632655419
C52	-3.0935409323	.1011448738	-1.1724703003
C53	-4.4500087679	-.2279120254	-1.2184069971
H54	-6.1002770724	-1.1509585030	-.1766705417
H55	-4.7212181461	-1.7328044656	1.8131336834
H56	-2.3374136959	-1.1495572449	1.8911271534
H57	-2.6579457257	.6284770646	-2.0174177217
H58	-5.0377274465	.0368528876	-2.0937946199